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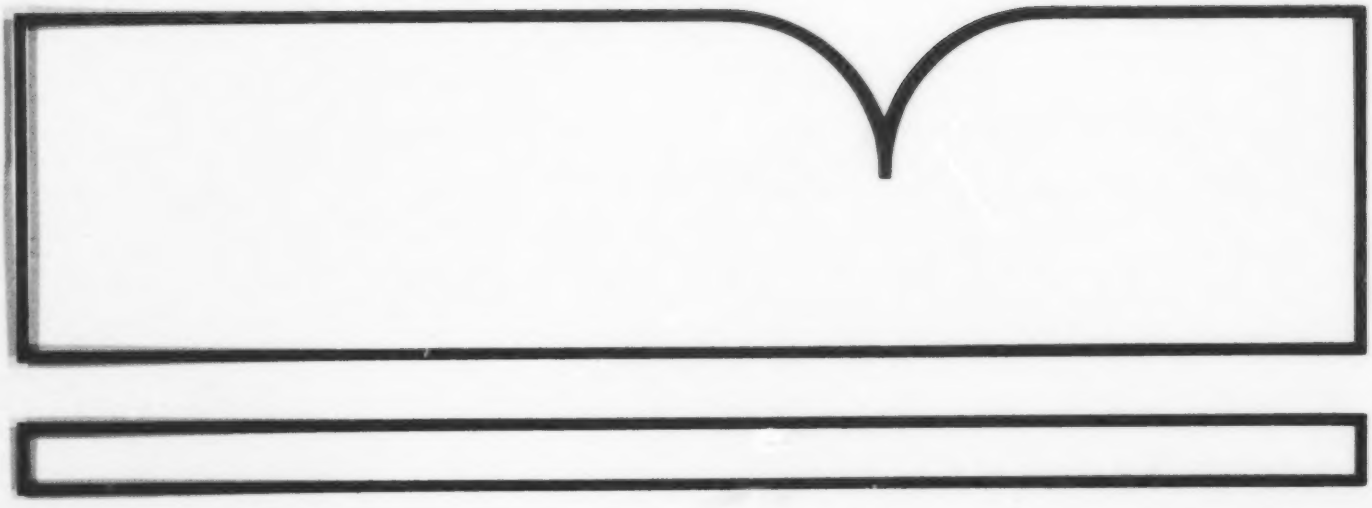

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EXPOSURE ASSESSMENT FOR THE PESTICIDE ALDICARB IN FLORIDA, USA

by

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ABSTRACT

In this paper, computer modeling work related to an exposure assessment for the pesticide aldicarb in the state of Florida, USA, is presented. The work was divided into two phases: deterministic modeling of contaminant transport under various soil/climate/management scenarios for both the unsaturated and saturated zones, and uncertainty analysis of transport in the unsaturated zone using Monte Carlo simulations. The paper briefly describes the modeling study, reports results of the unsaturated zone modeling and compares the loading estimates for aldicarb to groundwater utilizing both deterministic and probabilistic techniques.

BACKGROUND

The pesticide aldicarb is used extensively in Florida citrus for the control of nematodes and other pests. Evidence of aldicarb contamination in groundwaters of the state sparked public concern and prompted a March 1983 suspension of the use of the compound in all but three Florida counties. In September 1983, the use of aldicarb was reinstated with the restrictions that it would not be used within 90 m (300 ft) of drinking water wells and that application would be at half the label rate of 11.2 kg/ha.

In 1984, a modeling study was performed to assess aldicarb concentrations in drinking water wells in the vicinity of citrus groves (Dean and Atwood, 1985). The modeling study was part of a coordinated risk assessment conducted by the U.S. EPA. Areas in the citrus-growing region were identified, with respect to the unsaturated and saturated zones, in which fate and transport of aldicarb were thought to be uniquely different. An extensive literature search was conducted to determine degradation and transformation rates, and adsorption coefficients for aldicarb. These regional and chemical data were used to define various simulation scenarios. The fate and migration of aldicarb was then simulated in the unsaturated zone using PRZM (the Pesticide Root Zone Model; Carsel, et al., 1984) and in the saturated zone using CFEST (Combined Fluid-Energy-Solute Transport model; Gupta, et al., 1982). Continued interest in the problem lead to subsequent work in which the transport of aldicarb to groundwater was again modeled (using PRZM), this time taking into account uncertainty in the pesticide and soils parameters used as model coefficients.

The objectives of this paper are twofold - to briefly describe the modeling study and to answer two questions: what is the impact of making misjudgements about the mean values of model parameter, and, what is the impact of neglecting uncertainty in model parameter estimates?

ENVIRONMENTAL SETTING AND PESTICIDE CHARACTERISTICS

Environment

Citrus is grown throughout most of central and southern Florida (Figure 1). A great deal of fruit is grown in the "ridge" area, a region of sand hills running north-south in the center of the state, and in the "flatwoods" area, a region of lowlands which flank the ridge area on both the east and west coasts. In each of these areas, climate, soils, management practices, and thickness of the unsaturated zone can be quite different. These factors cause substantial differences in the fate and transport of aldicarb to groundwater.

Figure 1. *Subareas delineated for unsaturated zone modeling*

Critical climatic variables are precipitation and evaporation which determine the quantity of water available for percolation through the soils. In the soil, water content and saturated hydraulic conductivity, soil organic matter content, and soil pH are important factors. Water content and hydraulic conductivity determines the velocity at which water moves through the soil, while organic-matter content affects chemical adsorption, and pH strongly affects aldicarb degradation. Data analysis indicated that differences in these factors were pronounced among four soil orders on which citrus is grown in Florida: the entisols, ultisols, spodosols, and alfisols.

Based on climatic, soils, management, and physiographic considerations, the Florida citrus-growing region was subdivided into the six areas shown in Figure 1. Area 1 is an area of primarily ultisols, while area 2 consists primarily of entisols. Areas 3 and 5 consist primarily of spodosols, while areas 4 and 6 contain primarily alfisols. Management practices vary somewhat between these areas. Areas 5 and 6 receive about 10% more rainfall on an annual basis than areas 3 and 4.

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For the sake of brevity, only the results for unsaturated transport in thin ridge soils (i.e., ridge areas having a shallow groundwater table) are discussed in this paper. Loadings to groundwater are greatest in this area. The results of the deterministic modeling of all the unsaturated and saturated zone scenarios have been reported elsewhere (Dean and Atwood, 1985).

Pesticide Characteristics

Aldicarb is a nematicide, acaricide, and a systemic insecticide. Its environmental fate is dominated by two factors: it forms two toxic daughter products, and is highly mobile in soils. Degradation of the toxic residues of the compound is of intermediate duration compared to other pesticides. Aldicarb is rapidly oxidized to aldicarb sulfoxide, which in turn is more slowly oxidized to aldicarb sulfone. Concurrently, these three carbamates are transformed by hydrolysis to corresponding oximes. These products of hydrolysis are far less toxic than aldicarb, its sulfoxide or its sulfone, and are of little environmental concern. A schematic of these processes is shown in Figure 2. The chemistry and environmental fate of aldicarb have been described by a number of researchers. A thorough review of its properties has been compiled in Dean, et al., 1986.

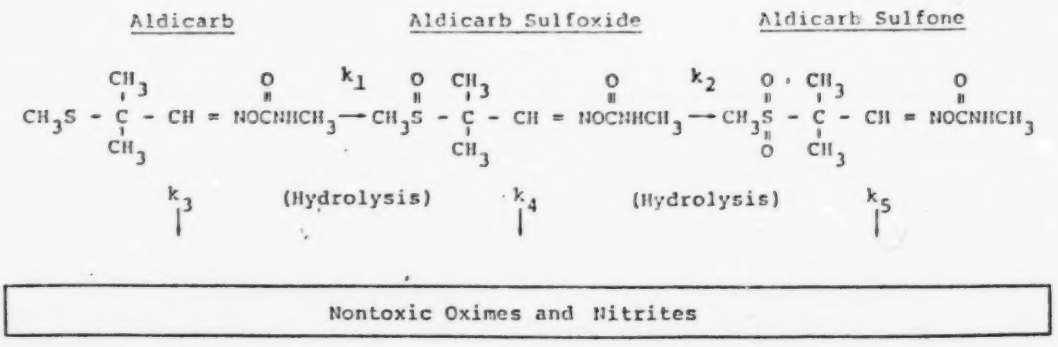

Figure 2. *Schematic of aldicarb environmental chemical pathways*

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MODEL IMPLEMENTATION

PRZM was modified in this study so that the transformation of aldicarb to its daughter products could be simulated in the unsaturated zone. Therefore, the rates k_1 through k_5 had to be estimated for each transformation/degradation pathway and adsorption partition coefficients had to be estimated for aldicarb, its sulfoxide, and its sulfone. This was accomplished by taking rates from the literature and regressing the values on concurrently measured variables such as pH, temperature, soil water content and organic matter. Rates were predicted for each modeling scenario using these regression equations and mean valued data on local soil conditions. Adsorption partition coefficients were determined using average values of K_{oc} found in the literature with localized values of soil organic carbon. Two parameter sets were derived by two independent groups of experts to evaluate the "accuracy" of the selected values.

Deterministic Approach

Mean values for pesticide parameters were estimated by experts from Syracuse Research Corporation (SRC) without knowledge of the values used in the 1984 modeling study. Deterministic model runs were then made to compare the output obtained using the two sets of mean valued input. Meteorological data from Lake Alfred, Florida was used to drive the model. Because a number of years were run, the output was summarized into frequency distributions of the annual leaching load.

Probabilistic Approach

One of the purposes of this study was to evaluate the impact of having expected uncertainty in the mean values of pesticide coefficients in the original (1984) modeling effort using PRZM. A classical method of doing this is by using Monte Carlo analysis. The Monte Carlo method and yields the distributions of model output variables.

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The variability of parameters was taken into account while utilizing the mean values of the parameters from the 1984 modeling study and the more recent SRC estimates. The parameters under consideration for the uncertainty analysis were the following:

- adsorption coefficients (K_{oc}) for each species (aldicarb, AS; aldicarb sulfoxide, ASO; and aldicarb sulfone, ASO_2),

- transformation rate constants ($AS \rightarrow k_1 \rightarrow ASO$, $AS \rightarrow k_2 \rightarrow ASO_2$),

- degradation (hydrolysis rate) constants (k_3, k_4, k_5), and

- soil parameters (pH, organic carbon, water holding capacity, bulk density).

Details of the parameter estimation process are given in Dean, et al., 1986. Results are reported in the following section.

The approach for performing the Monte Carlo analysis was designed to conserve computer time while providing the information necessary to answer the question posed above. Ideally, the way to perform the analysis would be to rerun each of the deterministic scenarios run previously, considering the uncertainty in climate as well as in pesticide parameters. This information could then be used to calculate an ensemble of frequency distributions of pesticide leaching loads. Confidence bands could then be calculated for each distribution. Projections of the computer time and budget required to do so showed this to be infeasible. Instead, the following approach was used. Values of pesticide loads were taken at the 90%, 50%, and 10% exceedance probability levels from the previously derived frequency distribution. For each of these "target" simulation loads, a year having an annual load closest to the target was selected. These three years were then used in the subsequent Monte Carlo simulations.

This approach has some distinct advantages and disadvantages. A definite advantage is the savings in simulation time. Only a fraction

of the original simulation years had to be rerun. Another advantage is that the variability in the output due to pesticide parameters (from single year Monte Carlo runs) versus meteorological variability (from multiple year deterministic runs) is differentiated. The variation in the original frequency distribution is due primarily to time variability in rainfall, evapotranspiration, and/or temperature, and secondarily to differences among scenarios in soils and management (e.g., irrigation practices). The variability in the ensemble runs generated about the old frequency curves at selected exceedence values, is due primarily to uncertainty in pesticide parameters. Although there was some statistical interaction between results, the two analyses should show the relative effects of variability of climatic factors versus pesticide properties. A disadvantage is that the distribution of the integrated effects of variability in climatic factors and uncertainty in pesticide parameters is not directly obtained.

SIMULATION RESULTS

The annual pesticide loading results for thin ridge soils from the 1984 modeling study is shown in Figure 3. The points in the distribution consist of results from simulations of both entisols and ultisols for all appropriate management factors considered. These results were found not to be significantly different statistically. By combining the simulation results from several scenarios, better estimates of the probabilities are obtained. The 90%, 50%, and 10% exceedance probability loads are 0.006, 0.04 and 0.3 kg/ha, respectively.

Table 1 shows a comparison of the results of deterministic runs and means from the Monte Carlo analyses. The first column shows the annual pesticide leaching loads from the original simulations for the years chosen to represent the 10, 50 and 90 percent exceedance levels. The second column shows the results of using values estimated by SRC for chemical parameters. For the 10% exceedance level, the load was slightly lower (0.29 kg/ha) than the original simulations (0.32 kg/ha). At the 50% exceedance level, the SRC output was lower by 37% and at the

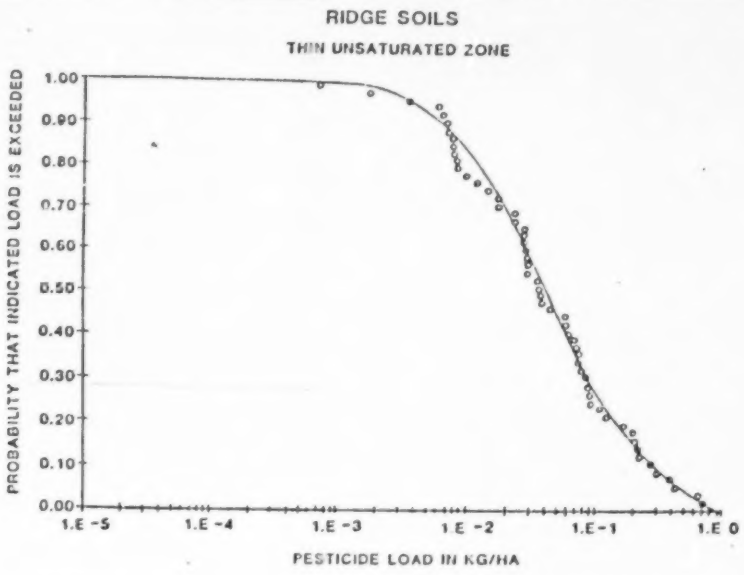

Figure 3. *Frequency of annual quantity of pesticide leached to the unsaturated zone from thin Entisols and Ultisols*

90% level, the SRC output was about one third of the original output (0.002 kg/ha versus 0.006). It is noteworthy that the results are most similar at higher loading values. This makes sense because the highest leaching loads occur in years in which large storms occur soon after application. Under these circumstances, degradation parameter selection is less likely to have an impact in the results.

Table 1. *Deterministic results, means and coefficients of variation from Monte Carlo simulations for thin ridge soils*[1]

	Deterministic Results		Monte Carlo Results		
Exceedance Level	Original Coefficients	SRC Coefficients	Original With Correlation	Original Without Correlation	SRC With Correlation
0.10	0.320	0.29	0.78	0.72	0.63
			(70.5)	(80.5)	(107.9)
0.50	0.038	0.024	0.24	0.20	0.22
			(79.2)	(95.0)	(159.1)
0.90	0.006	0.002	0.065	0.065	0.049
			(109.2)	(153.8)	(244.5)

[1] Units are kg/ha

Table 1 also shows the results of Monte Carlo simulations. Three cases were run: Dean and Atwood (original) parameters both with and without estimated correlation among inputs, and SRC parameters with correlation. The values shown in the table are the ensemble means of 200 simulations for each case. The parenthetic numbers are corresponding coefficients of variation (expressed as percents) for each case.

Because of the uncertainty in the estimates of correlation coefficients, Monte Carlo simulations were performed both with and without correlation. As can be seen in Table 1, correlation produced slightly higher mean responses and slightly lower coefficients of variation than when correlation was not considered.

The effect of considering uncertainty in pesticide parameters used in the original simulations PRZM was to increase the mean annual leaching output. The mean response for the thin ridge soils at the 10% exceedance level increased by a factor of 2.4 over the original output of 0.32 kg/ha. At the 50% exceedance level, the response increased by a factor of 6.3 over the original output of 0.038 kg/ha. At the 90% exceedance level the mean increased over an order of magnitude.

As in the case just discussed, consideration of uncertainty with SRC parameter estimates produced higher ensemble mean responses than the corresponding deterministic outputs. SRC parameters produced outputs with slightly lower means than the simulations produced with the original parameter set. However coefficients of variation were higher with the SRC parameter set.

These analyses have demonstrated that although the leaching output produced by PRZM is sensitive to chemical parameters, the difference in results produced by data sets derived independently by two groups of experts was small. However, consideration of the variability in parameter estimates can have dramatic results on the leaching output produced. Results were relatively insensitive to estimates of parameter covariance.

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